Green Function Theory of Ferromagnetism*

by

Vinod Mubayi and Steve P. Heims

Brandeis University

In the theory of the Heisenberg ferromagnet, the Green function technique has provided an interpolation scheme which gives useful results for the thermodynamic behavior of the quantities of interest, like the magnetization, the specific heat and the susceptibility in all temperature ranges. So far the main attempt in the Green function approach has been to try to discover ingenious methods of decoupling the higher order Green function to obtain better agreement with rigorous spin wave theory at low temperatures. In the region of the Curie point, most of the decouplings studied so far give the same qualitative results as the molecular field theory. Our approach is to try and see whether it is possible, without an explicit decoupling approximation, to obtain, within the Green function formalism, a connection between the quasi-particle spectrum and the critical behavior. In particular, we examine the implications of a cube-root behavior of the magnetization near the Curie point, as suggested by the experiments of Heller and Benedek, on the form of the quasi-particle spectrum and the behavior of the specific heat.

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* Work supported by NASA G-612

Read at APS meeting, New York: Bull. Am. Phys. Soc. 11, 387 (1966)

We define the retarded Green function

(1) $$G^{ret}_{gf}(t) = -i\,\theta(t)\langle[S^+_g(t)\,,\,S^-_f(0)]\rangle$$ in the usual notation. Going to reciprocal lattice space we have the conditions

(2) $$G^{ret}_k(t)\big|_{t=0^+} = -i\;2\langle S^z\rangle$$ independent of k

(3) $$i\frac{d}{dt}G^{ret}_k(t)\big|_{t=0^+} = \alpha_k\,,$$ a quantity which can be obtained from the Heisenberg equations of motion.

In general,

(4) $$G^{ret}_k(t) = \theta(t)\int A_k(\omega_k)\,e^{-i\omega_k t}\,d\omega_k$$

Then the conditions (2) and (3) imply the following sum rules

(5) $$\int A_k(\omega_k)\,d\omega_k = -i\;2\langle S^z\rangle$$

(6) $$\int \omega_k A_k(\omega_k)\,d\omega_k = \alpha_k$$

So far everything is quite general. We now consider the case $A_k(\omega_k) = A\delta(\omega_k - E_k)$ where E_k are the energies of the elementary excitations (or quasi-particles) of the system. This choice of $A_k(\omega_k)$ corresponds to the assumption that a description of the system in terms of quasi particles with sharply defined energies (i.e. no damping) is valid. Equivalently, in terms of decouping of the higher order Green function $G_2 = \Sigma G_1$ it implies that the mass operator Σ does not have a complex part (though it may have an anomalous structure as indicated by Wortis).

Now with the choice

(7) $$G^{ret}_k(t) = -i\,\theta(t)\;2\langle S^z\rangle\;e^{-iE_k t}$$

and the conditions (1) and (2) it can be shown that for a cubic lattice with only nearest neighbor interactions the k-dependence of E_k is $E_k \sim [1 - \frac{1}{z}\,\Sigma_\delta\,e^{-i\,\underline{k}\cdot\underline{\delta}}]$. For definiteness we consider

consider the case of spin one-half and write $\sigma = 2\langle S^z\rangle$. In general the spectrum can be taken to have the form

$$E_k = F(\sigma)\left[1 - \frac{1}{z}\sum_\delta e^{-i\underline{k}\cdot\underline{\delta}}\right] \tag{8}$$

If we write $F(\sigma)$ as a general power series in σ, $F(\sigma) = \sum_n a_n \sigma^n$, in order for a phase transition to occur only positive powers of σ must enter. The magnetization is given by the expression

$$\frac{1}{\sigma} = \frac{\Omega}{(2\pi)^3}\int d^3k \coth\beta\frac{E_k}{2} \tag{9}$$

Near the Curie point since σ is small an expansion in powers of σ is meaningful. Expanding the coth one obtains an expression of the form

$$1 - \frac{T}{T_c} = \sum_m b_m \sigma^m$$

where the b_m are related to the a_n. It turns out that a_1 is directly related to T_c; if $a_2 \neq 0$ we get a linear dependence of σ on $1 - \frac{T}{T_c}$; if we choose $a_2 = 0$ then we have a square root dependence of σ on $1 - \frac{T}{T_c}$ unless $a_3 = \frac{4F^2(-1)}{6\beta_c}$ where $F(-1)$ is the well-known Watson sum; with this choice of a_3 we get

$$\sigma = \text{const.}\left(1 - T/T_c\right)^{\frac{1}{3}} \tag{10}$$

which is suggested strongly by available experiments. The proportionality constant is directly related to a_4 and can be used to determine a_4 empirically.

If with this spectrum we now evaluate the specific heat, we find

$$C_H \sim \left(1 - \frac{T}{T_c}\right)^{-\frac{1}{3}} \qquad \text{for} \quad T \lesssim T_c$$

Experimentally, however, the singularity in the specific heat is indicated to be logarithmic. Since the only approximation in our analysis consisted of a choice for the form of A_k (ω_k) in the Green function we conclude that a different form of $A_k(\ _k)$ which may possibly, include damping effects is necessary; a quasi stationary description is not valid in the critical region.

To make a similar analysis for spectra with a finite width we should use a third sum rule

(11) $$\frac{d^2 G_k^{ret}(t)}{dt^2}\bigg|_{t=0^+} = \int \omega_k^2 \, A_k(\omega_k)\, d\omega_k$$

We have not yet made this analysis but we can make some preliminary observations for some definite line shapes.

For a Lorentzian line we find

(12) $$\frac{1}{\sigma} \sim \int d^3k \, \frac{E_k}{E_k^2 + \Gamma_k^2} \qquad + \text{ finite terms}$$

So the singularity can come only from the region $E_k \rightarrow 0$ and $\Gamma_k \rightarrow 0$ which appears inconsistent with the observation of line-broadening near the critical point. However, if the line shape is a function of ω_k with discontinuities or even discontinuous first derivatives a singularity will arise from finite values of E_k. For example, a rectangular pulse centered at E_k of width Γ_k yields

(13) $$\frac{1}{\sigma} \sim \int \frac{d^3k}{2\beta\Gamma_k} \log \left| \frac{\sinh(E_k + \Gamma_k/2)}{\sinh(E_k - \Gamma_k/2)} \right|$$

which has a singularity at $E_k = \Gamma_k/2$

Finally, we mention briefly a parameter dependent decoupling similar to the one employed by Callen in which we tried to make use of the condition (3) on $i\frac{d}{dt}G_k$ already mentioned in order to obtain a self-consistent expression for the parameter and the energy E through use of the fact that $i\frac{d}{dt}G_1$, is related to G_2. In RPA the two ways of calculating the energy give different results. The higher-order Green function G_2 was decoupled as follows:

$$G_{pg,f} = \{\alpha_{pg} + (1-\alpha_{pg})\bar{n}\} G_{gf} - \alpha_{pg} \langle S_p^- S_g^+ \rangle G_{pf} \tag{14}$$

where $\bar{n} = \frac{1}{2} - \langle S^z \rangle$ for the case of spin one-half. For a cubic lattice with nearest neighbor interactions one obtains through the self consistency procedure outlined

$$E_k = f(\mu,\sigma)\left[1 - \frac{1}{z}\sum_\delta e^{-i\underline{k}\cdot\underline{\delta}}\right] \tag{15}$$

where $\sigma = 1 - 2\bar{n}$ is the magnetization and $\mu = \langle S_p^- S_{p+\delta}^+ \rangle$ is related to the short range order in the system. $\sigma(T)$ and $\mu(T)$ are then obtained through a self consistent solution of the coupled equations

$$\frac{1}{\sigma} = \frac{\Omega}{(2\pi)^3}\int d^3k \coth \beta\frac{E_k}{2} \qquad \frac{\mu}{\sigma} = \frac{1}{2}\frac{\Omega}{(2\pi)^3}\int d^3k\, e^{i\underline{k}\cdot\underline{\delta}} \coth \beta\frac{E_k}{2} \tag{16}$$

At low temperatures, we evaluated $\sigma(T)$ and found it to be close to the RPA result, the T^3 term being still present. However, this decoupling does not have a finite Curie temperature similar to the result of Oguchi and Honma. The only way a singularity can arise for finite temperature is from E_k going to zero and it turns out from the form of $f(\mu,\sigma)$ that this implies that both σ and μ should go to zero at the same finite temperature. This is not only unphysical, for we expect some short range order to be present at the critical point, but also leads to an inconsistency.